IUCLID 5
Guidance and support

Installation Guide for IUCLID 5.4
Client-Server Architecture

Microsoft® Windows®

July 2012

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Chapter 1. Introduction

IUCLID 5 can be installed as standalone or in a distributed (multi-user) environment. This document describes how to install and configure the IUCLID 5 application in a distributed Microsoft® Windows® environment. If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting the ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

1.1. Hardware requirements

The server hosting IUCLID 5 must have at least:

- RAM: At least 2 GB on the mother board; 4 GB if PostgreSQL is run on the same machine as IUCLID 5
- Hard disk space: 200 GB
- CPU: Intel Pentium Dual @ 1.8 GHz
- Network adapter 100 Mbps (recommended 1Gbps)

The requirements depend in part on the plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database.

1.2. Software requirements

Operating system:

- Microsoft® Windows® Server 2003. Other versions (2000, XP, 2008) may be used, but note that the testing has been done with 2003.

IUCLID 5 can be installed with the following open source components:

- JDK 1.6. Installation packages can be downloaded from the site http://www.oracle.com.

Note

This is not the most recent version of Java.

- Tomcat 5.5.x or 6.0.x (where x is the latest version). Installation packages can be downloaded from http://tomcat.apache.org
- PostgreSQL 8.2, 8.3, 8.4 or 9.0 (recommended). Installation packages can be downloaded from http://www.postgresql.org

As an alternative to the free database software PostgreSQL, the commercial database software Oracle, can be used. You do not need both PostgreSQL and Oracle:

- Oracle® 10g or higher. Installation packages can be downloaded from http://www.oracle.com

  The Oracle driver for Java is no longer supplied with the IUCLID installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Java 1.6 and Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`. For use with Tomcat, the driver must be placed in Tomcat's library folder, e.g. `Tomcat\lib`.

The following essential components can be downloaded without charge from the IUCLID 5 web at the at http://iuclid.eu. Before downloading them, you must register as a user on the site.

- The IUCLID 5 distributed installation package, version 5.4.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID 5 web site where the installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory, which are also available from the web site http://iuclid.eu.

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set,* a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

For more information regarding system requirements, see the FAQ on the IUCLID web site located at http://iuclid.eu.

Chapter 2. Making a fresh installation of IUCLID 5

The following chapter contains a brief description of the actions required to make a fresh installation of IUCLID 5 that runs within a web server on Windows.

2.1. Operating System

IUCLID 5 has been tested using Windows Server 2003. Other versions (2000, XP, 2008) may be used as well. In that case the file locations might differ from those used in this document. For installation instructions, please refer to the documentation supplied by the manufacturer.

2.2. JAVA Development Kit

Download the JAVA Development Kit (JDK) 6 or JAVA Runtime Environment (JRE) 6 according to the architecture of the destination computer from the site http://www.oracle.com. [http://www.oracle.com] Run the installer and follow the instructions. The default parameters are appropriate for IUCLID 5. For more information, please refer to the documentation on the site from which the software is available.

2.3. Database - PostgreSQL

PostgreSQL is an open source, object-relational database system. Installation packages, and more information about the software can be obtained from the site http://www.postgresql.org.

2.3.1. Installation of PostgreSQL

If either version 8.2, 8.3, 8.4 or 9.0 of PostgreSQL is already installed and running as a service with a user `postgres`, the existing installation can be used. There is no specific need to upgrade to a higher version number. If PostgreSQL is not already installed on the computer, or you would like to upgrade it, download the new version of PostgreSQL from the site www.postgresql.org/download and install it. The web site of PostgreSQL offers a range of alternative ways to download and install the PostgreSQL software. The screen shots shown below show the use of the *one click installer* available from the PostgreSQL web site. An example of the file name of the installer is *postgresql-9.0.4-1-windows.exe*.

The default fresh installation of PostgreSQL, made using the *one click installer*, automatically starts PostgreSQL as a service, creates the user `postgres` if necessary, and supplies administration tools (e.g. pgAdmin III) that can be used to manage databases. If the installer creates the database superuser `postgres`, you will have to enter a password for it into step 4 of the *one click installer*, as shown in the sequence of figures below. Remember this password because it will be required later, during the configuration of IUCLID 5. If you are unsure of what values to enter into the *one click installer*, use the pre-filled defaults.

Figure 2.1. Installer for PostgreSQL

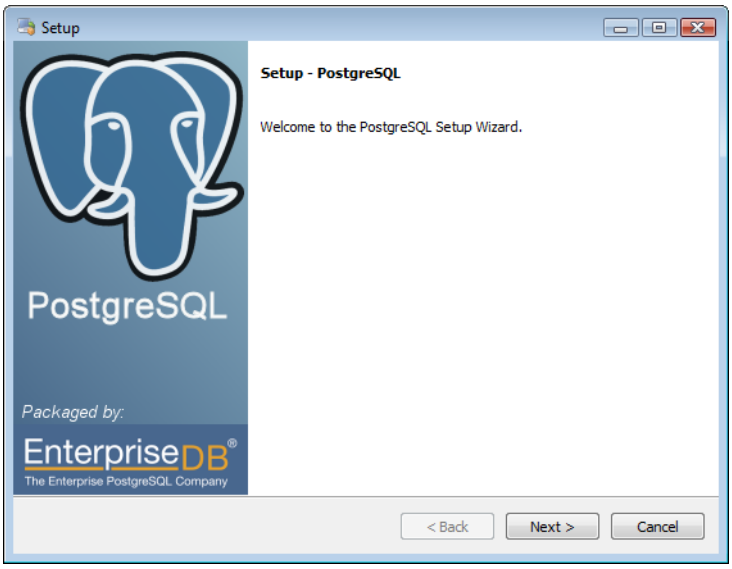


Figure 2.2. Installation directory for PostgreSQL

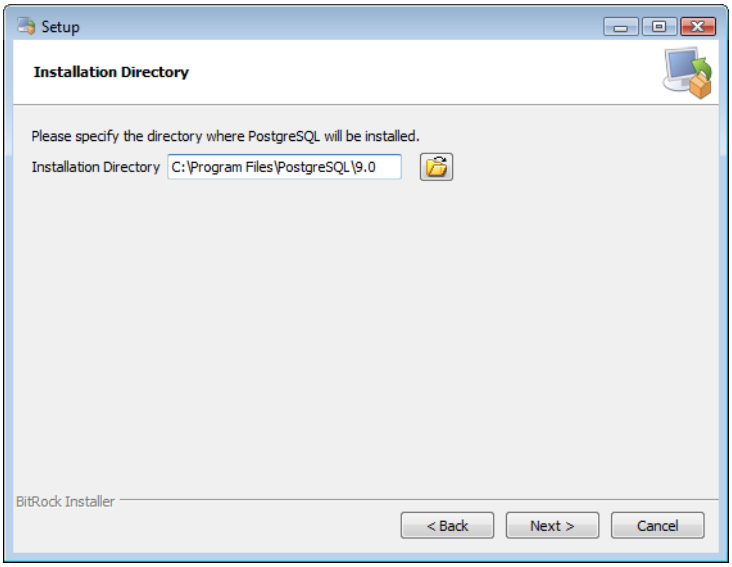


Figure 2.3. Data directory for PostgreSQL

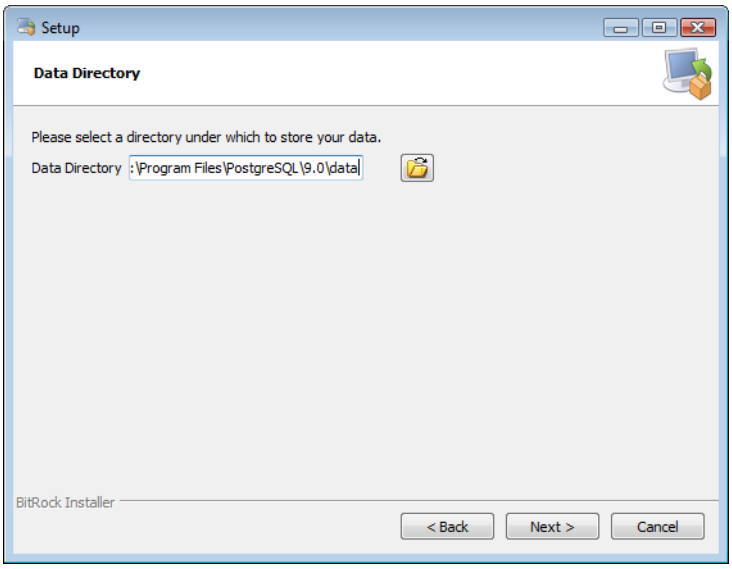


Figure 2.4. Password for the database superuser (postgres) and the Windows service account (postgres)

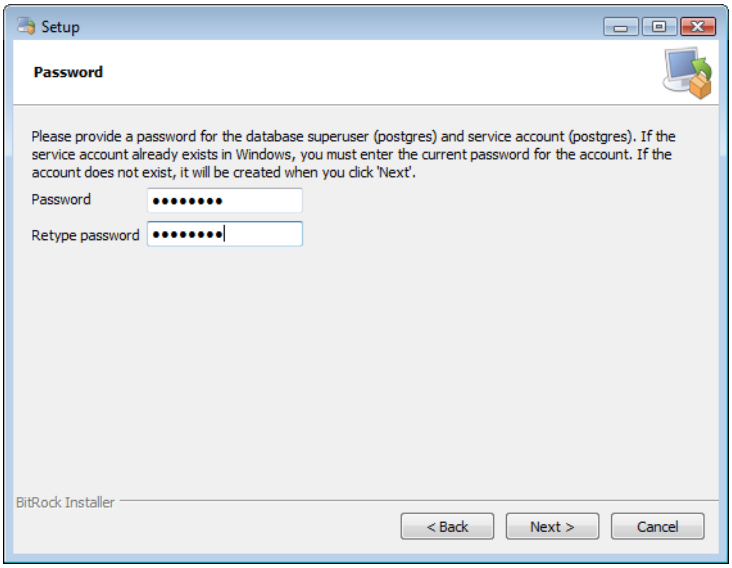

Setup
Password
Please provide a password for the database superuser (postgres) and service account (postgres). If the service account already exists in Windows, you must enter the current password for the account. If the account does not exist, it will be created when you click 'Next'.
Password
Retype password
BitRock Installer
< Back
Next >
Cancel

Figure 2.5. Port number for PostgreSQL

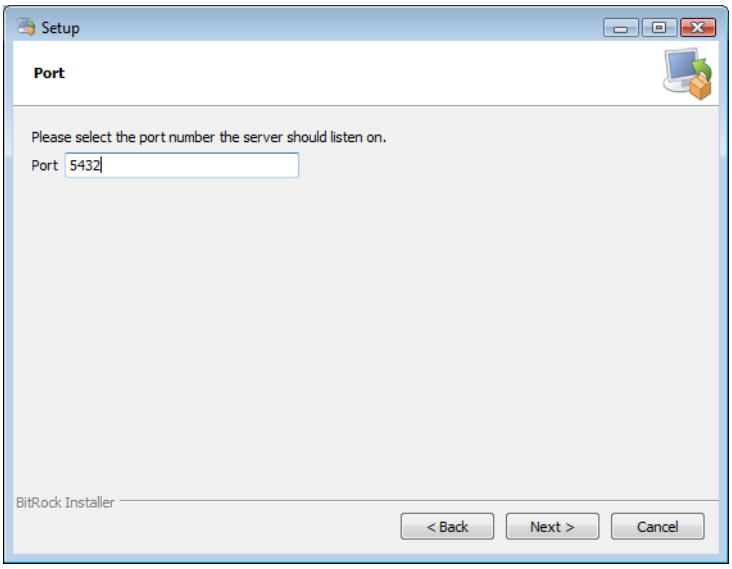


Figure 2.6. Set the default locale for PostgreSQL

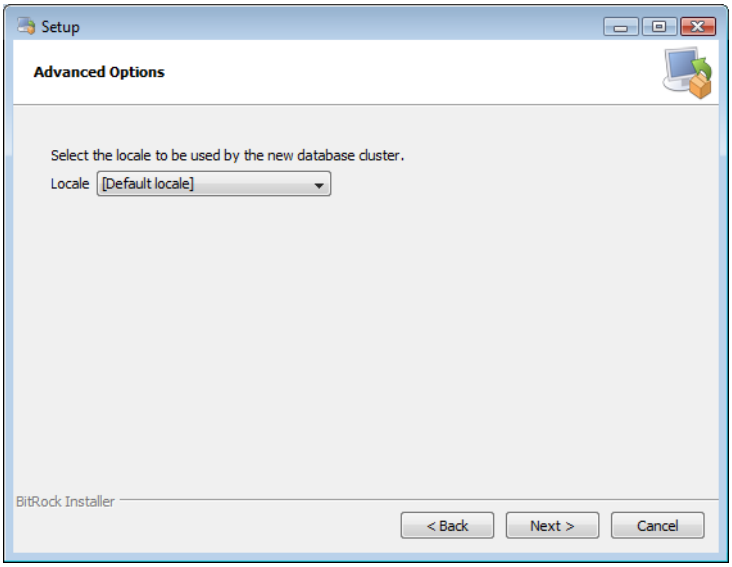


Figure 2.7. Confirm installation of PostgreSQL

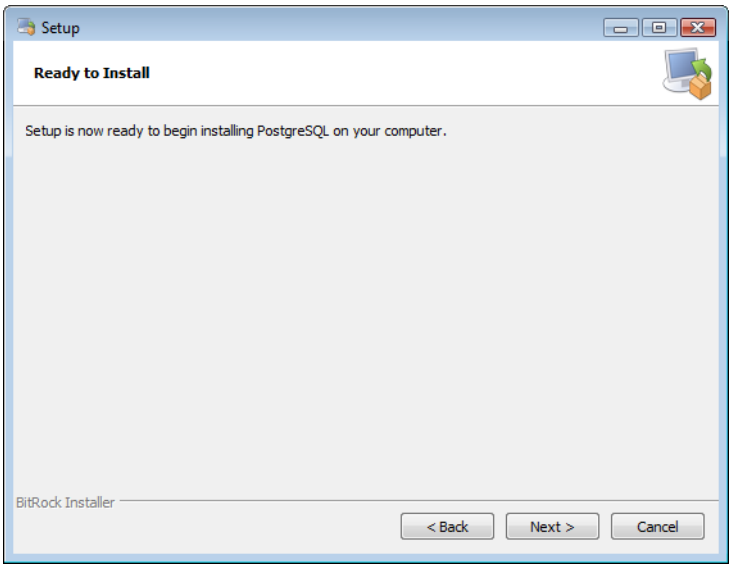


Figure 2.8. Installation of PostgreSQL in progress

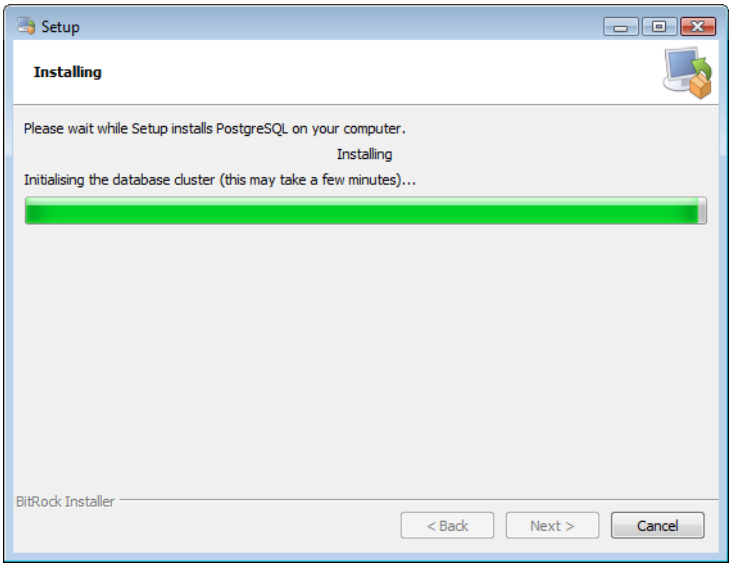


Figure 2.9. Installation of PostgreSQL complete

Setup
Completing the PostgreSQL Setup Wizard
Setup has finished installing PostgreSQL on your computer.
Launch Stack Builder at exit?
Stack Builder may be used to download and install additional tools, drivers and applications to complement your PostgreSQL installation.
PostgreSQL
Packaged by:
EnterpriseDB
The Enterprise PostgreSQL Company
< Back
Finish
Cancel

Unless you particularly want to run the Stack Builder, untick the box in the screen shown above. To finish the installation, click on the button Finish.

2.3.2. Configuration of PostgreSQL

A new user and a new database need to be created.

Tip

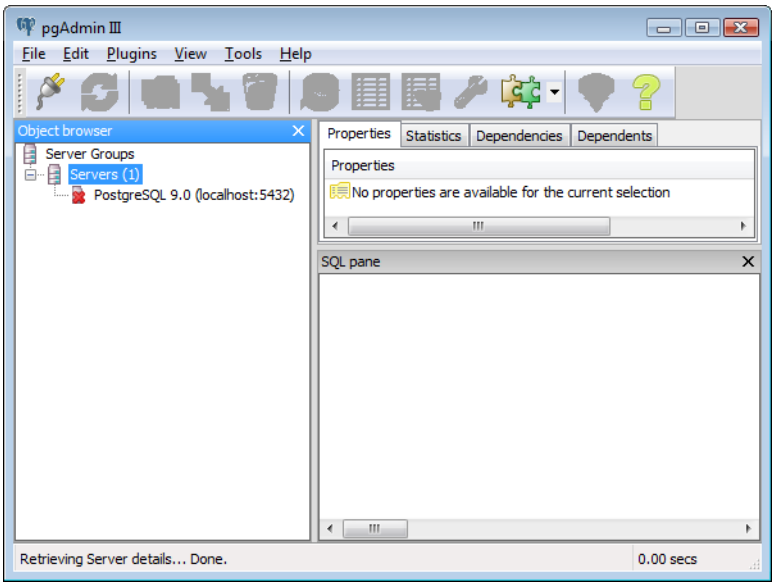
IUCLID 5 is configured by default to connect to the database using username:*iuclid5* and password:*iuclid5*. It is convenient to specify the same password now, and change it later when the application is set up correctly.

Important

Take note of the password of this user. This user name and password will be needed later to connect IUCLID 5 to the database.

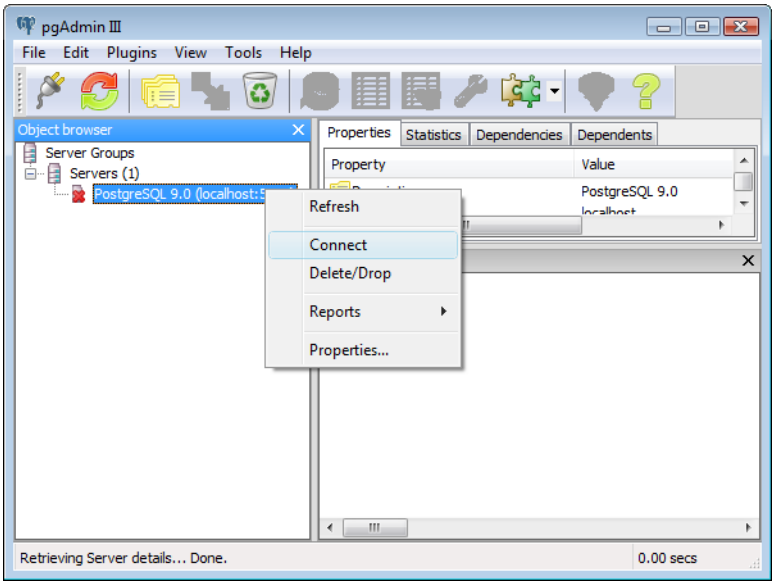
The program pgAdmin III can be used to create the database as follows. Start pgAdmin III from the menu *Start / All Programs / PostgreSQL9.0*. After the splash screen has appeared and you have closed the pop-up window that shows usage tips, the following screen is shown.

Figure 2.10. pgAdmin III interface on first opening



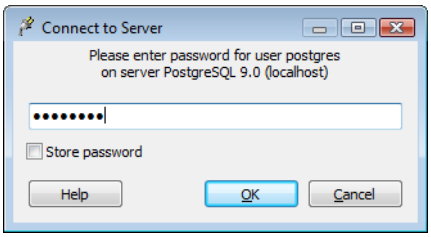
Right-click the text *PostgreSQL 9.0 (localhost:5432)* that is under the word *Servers* highlighted in blue in the figure above. Select *connect* as shown below.

Figure 2.11. Connect pgAdmin III to PostgreSQL as user postgres



Enter the password for user *postgres* as given in the postgres installer Figure 2.4, “Password for the database superuser (postgres) and the Windows service account (postgres)” then click *OK*. It is recommended to store the password to facilitate future access.

Figure 2.12. Authenticate the user postgres



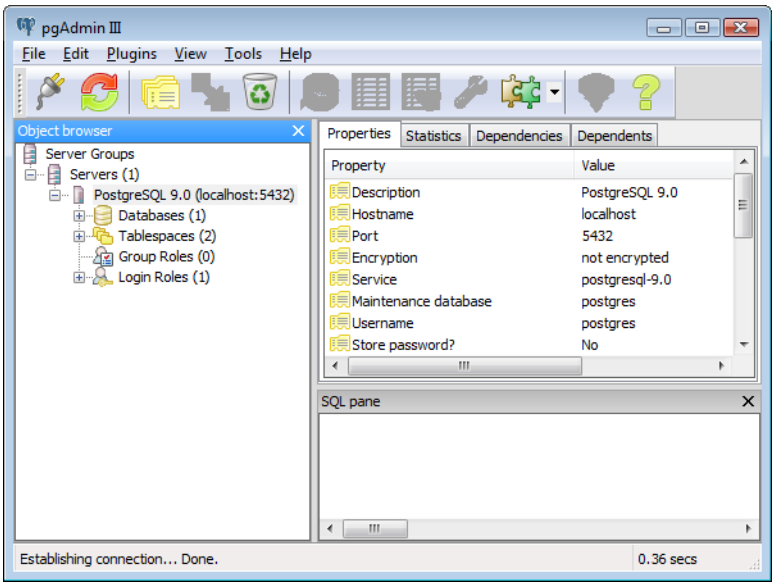
If you elect to save the password, the following warning might be displayed. Click *OK*

Figure 2.13. Saving passwords Warning

Guru Hint - Saving passwords
Saving passwords
WARNING: You have opted to save your password. It will be stored in plain text in your home directory on *nix systems, or in your user profile on Windows. If you do not want this to happen, please press the Cancel button.
pgAdmin uses PostgreSQL's 'pgpass' mechanism to store your passwords. On *nix systems, the password will be stored in ~/.pgpass, whilst on Windows systems it will be stored in %APPDATA%\PostgreSQL\pgpass.conf (%APPDATA% is the 'Application Data' folder in your user profile). This mechanism is used by default by all programs that use the libpq library to access the server, which includes command line applications such as pg_dump and pg_restore, other GUI applications, and drivers such as psqlODBC. This means that those applications may automatically connect to the server using your stored password. If you do not want this to happen, you should not use the Store Password option in pgAdmin.
Do not show this hint again
Help
OK
Cancel

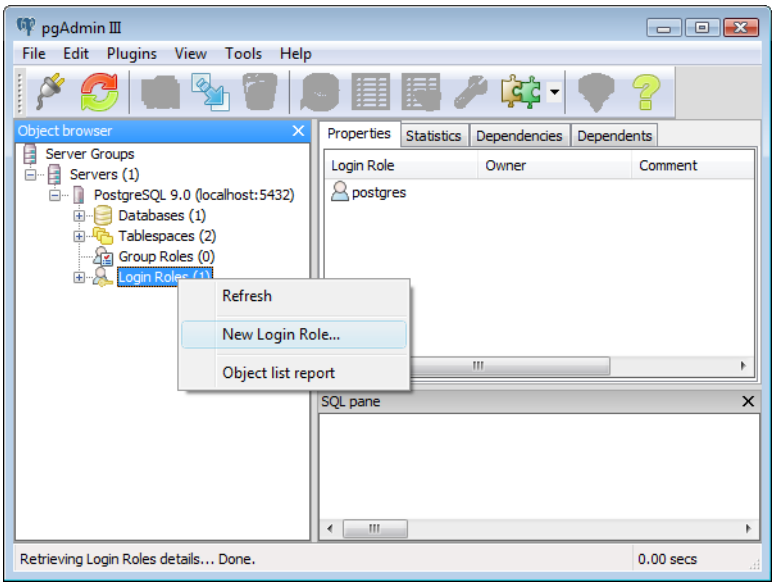
Expand the tree for *PostgreSQL 9.0 (localhost:5432)* by clicking the plus sign that has just appeared next to it, as shown in the figure below.

Figure 2.14. Initial screen in pgAdmin III



Right-click on *Login Roles* and select *New Login Role...*.

Figure 2.15. Select create a new user option

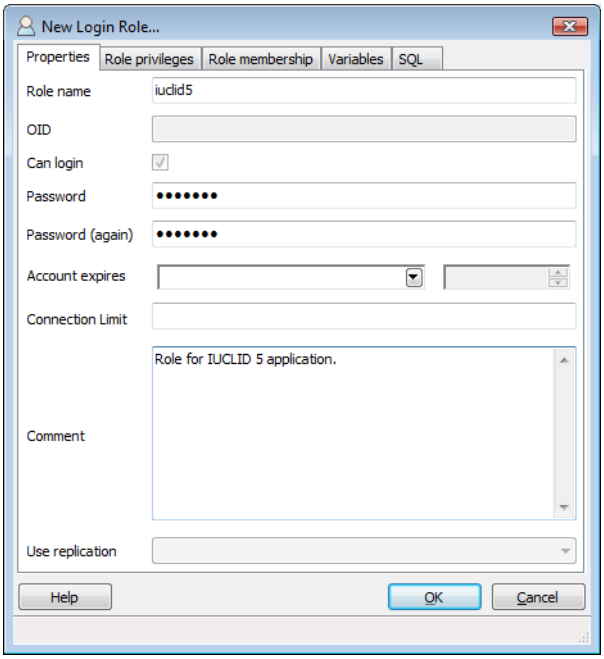


Enter the role name *iuclid5*. Set the password.

Important

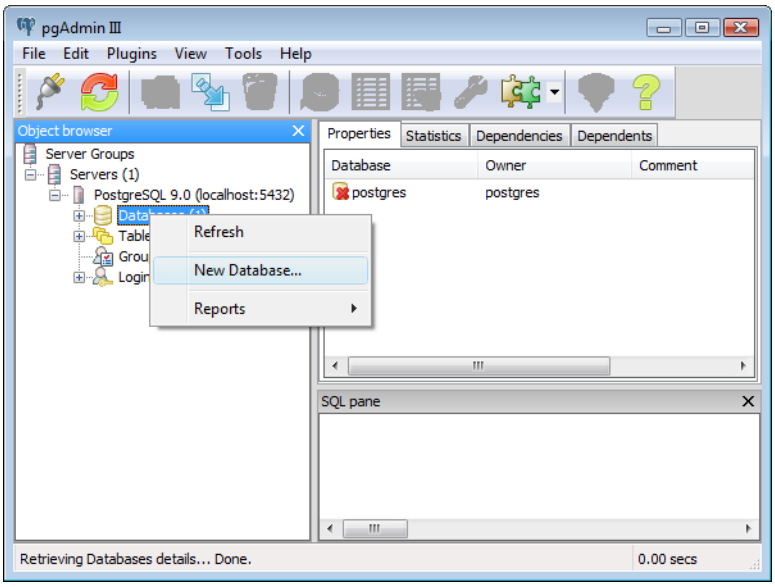
Make a note of the user name and password. They are referred to later in the installation, in Section 2.6.1, “Database connection settings for PostgreSQL”. We recommend using `iuclid5` as both the user name and the password.

Figure 2.16. Create a new role (i.e. a user) with the name iuclid5



Request a new database by right-clicking the text *Databases* and selecting *New Database...* as shown in the figure below.

Figure 2.17. Request a new database in pgAdmin III

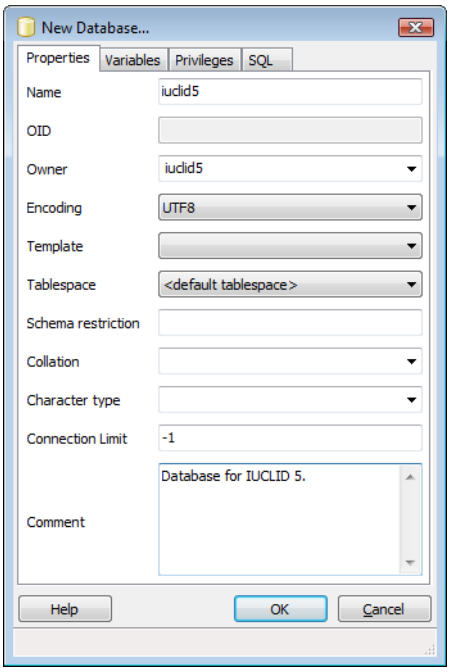


Enter the details you require. Normally these are only name=iuclid5 and owner=iuclid5. The encoding should be UTF8. Click *OK*.

Important

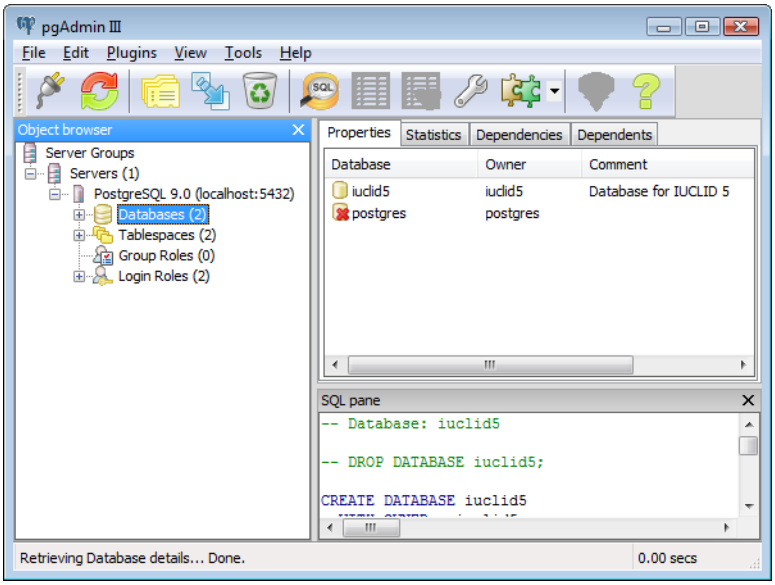
Make a note of the database name. It is referred to later in the installation, in Section 2.6.1, “Database connection settings for PostgreSQL”. We recommend using the name `iuclid5`.

Figure 2.18. Enter the details of IUCLID 5's database into pgAdmin III



As you can see from the figure below, there is now a new database named *iuclid5*.

Figure 2.19. List of databases in pgAdmin III



You can now close *pgAdmin III* and move directly to the installation of IUCLID 5.

2.4. Database - Oracle

The installation details of the Oracle DBMS are out of scope of this document due to its complexity. Please refer to the Oracle documentation or contact the vendor of the software.

However, the installation of `sqlplus` is described. `sqlplus` is the sql client application of Oracle (see below). It is needed to prepare a database for IUCLID 5 if Oracle is not installed on the computer where you are installing IUCLID.

2.4.1. Block size in Oracle

The default value of `block size` for an installation of Oracle is 8 KB. It is possible that a data field in IUCLID contains more data than is allowed for a block size of 8 KB. If this occurs, when an attempt is made to write the data to the database, the following error is generated: ORA-01450: maximum key length (6398) exceeded. To greatly reduce the chances of this error occurring, set `block size` to 16 KB. See the FAQ on the IUCLID web site for more detail.

2.4.2. Important technical information about existing IUCLID 5.x installations with Oracle

Ensure that the IUCLID 5 database user iuclid5 has not been granted with the **SELECT ANY TABLE** privilege, a DBA role, or direct **SELECT** grants to the secondary (iuclid5) database user tables, but only the privileges shown below in the SQL script. If you have granted extra privileges to the user iuclid5, you need to revoke these additional privileges, by, for example, logging in as `SYSTEM` and entering one or both of the following commands:

REVOKE CREATE SESSION FROM iuclid5;

REVOKE SELECT ANY TABLE FROM iuclid5;

The first denies access to database whereas the second denies access to the tables.

In order to successfully install IUCLID 5, follow the procedure below.

1. Logon to the Oracle database as `SYSTEM` or `SYSDBA`.

2. Create the new tablespaces and user iuclid5 as shown in the script below.
3. Test the user connection with the command: **connect iuclid5/iuclid5@10.1.14.27/IUCLID5**
4. If a previous version of IUCLID 5 is already deployed in the web application server, undeploy it.
5. Stop the web application server.
6. Copy the new .war file in to the folder `webapps`.
7. Start the application server. This deploys the application.
8. Stop the web application server.
9. Change the database connection string in the file `server.properties` to suit the target system.
10. Start the web application server.
11. Log in to IUCLID 5 using the account with name SuperUser and password root.
12. Import the backup you made with the backup plugin tool.

The following SQL script creates a user and an empty tablespace for IUCLID 5:

```
CREATE tablespace iuclid5_ts
 datafile 'iuclid5_ts.dbf' /*specify absolute path*/
 size 500M
autoextend ON
 next 500M
maxsize 2000M;


grant CREATE session TO iuclid5 identified BY "iuclid5";
grant CREATE TABLE TO iuclid5;
grant CREATE VIEW TO iuclid5;
grant CREATE sequence TO iuclid5;
ALTER USER iuclid5 quota unlimited ON iuclid5_ts;
ALTER USER iuclid5 DEFAULT tablespace iuclid5_ts;
```

2.4.3. Installing sqlplus

If Oracle is not installed on the computer where you are installing IUCLID then you need to install `sqlplus`, the sql client application of Oracle.

Download `instantclient-basic` and `instantclient-sqlplus` packages from http://www.oracle.com/technology/software/tech/oci/instantclient/index.html.

Install the packages using `rpm`, or unzip the packages if you have a 64 bit platform (replace the version according to the downloaded files).

```
~#rpm -iv oracle-instantclient-basic-10.2.0.3-1.i386.rpm \
oracle-instantclient-sqlplus-10.2.0.3-1.i386.rpm
Preparing packages for installation...
oracle-instantclient-basic-10.2.0.3-1
oracle-instantclient-sqlplus-10.2.0.3-1
~#
```

Set the environment variable LD_LIBRARY_PATH to the lib directory of Oracle.

```
~#export LD_LIBRARY_PATH=/usr/lib/oracle/10.2.0.3/client/lib
~#
```

Test the installation of sqlplus without connecting it to a database. If the SQL prompt is displayed, you have successfully installed the application. Close the program with the exit command.

Note

If an error message is displayed when you start sqlplus, check that the environment variable LD_LIBRARY_PATH points to the correct directory.

```
~#sqlplus /NOLOG
SQL*Plus: Release 10.2.0.3.0 - Production on Mon May 14 11:56:03 2007
Copyright (c) 1982, 2006, Oracle.  All Rights Reserved.
SQL>exit
~#
```

For more information on Instant Client, see the official Instant Client site at http://www.oracle.com/technology/tech/oci/instantclient/instantclient.html.

2.4.4. Preparing the tablespace

In order to create a new tablespace and user you have to log in as SYS user. If you do not know the SYS password ask your Oracle database administrator to create the iuclid5 user and tablespace.

Start sqlplus and connect to Oracle as a system administrator.

```
~#sqlplus /NOLOG
SQL*Plus: Release 10.2.0.3.0 - Production on Mon May 14 11:56:03 2007
Copyright (c) 1982, 2006, Oracle.  All Rights Reserved.
SQL>connect SYS/syspassword@servername/databasename AS SYSDBA
Connected.
SQL>
```

IUCLID 5 requires the UTF-8 default character set of the database. Execute the following select command in order to check the character set of the current database.

```
/* checks the characterset of the current database */
SQL>select property_value from database_properties
where property_name='NLS_CHARACTERSET';

PROPERTY_VALUE
--------------------------------------------------------------------------------
AL32UTF8
```

The default character set must be "AL32UTF8". If your setting is different, ask the database administrator to create a new database specifying AL32UTF8 as the default character set.

Create the iuclid5 user and tablespace in the database. It requires the password to be changed.

```
/* These SQL commands create a user and an empty tablespace for IUCLID 5 */
SQL>create tablespace iuclid5_ts
 datafile 'iuclid5_ts.dbf' /* specify absolute path */
 size 500M
 autoextend on
 next 500M
 maxsize 2000M;

Tablespace created.

SQL>grant create session to iuclid5 identified by "CHANGEIT";
Grant succeeded.

SQL>grant create table to iuclid5;
Grant succeeded.

SQL>grant create view to iuclid5;
Grant succeeded.

SQL>grant create sequence to iuclid5;
Grant succeeded.

SQL>alter user iuclid5 quota unlimited on iuclid5_ts;
User altered.

SQL>alter user iuclid5 default tablespace iuclid5_ts;
User altered.

SQL>
```

Disconnect from the database.

```
SQL>disconnect
Disconnected from Oracle Database 10g Release 10.1.0.3.0 - 64bit Production
SQL>
```

2.4.5. Checking the iuclid5 database user

Connect to the database using the username and password of iuclid5 in order to verify that the database server accepts a connection made by iuclid5 user.

```
SQL>connect iuclid5/i5password@servername/databasename
Connected.
SQL>exit
~#
```

Warning

Do not start IUCLID 5 until you successfully connect to Oracle using sqlpus from the server hosting IUCLID 5 web application.

2.4.6. FAQ

If you want to delete the previously created user and tablespace, connect to Oracle as sysdba and execute the `drop user` and `drop tablespace` commands.

```
SQL>connect SYS/syspassword@servername/databasename AS SYSDBA
Connected.
SQL>drop user iuclid5 cascade;

User dropped.

SQL>drop tablespace iuclid5_ts including contents and datafiles;

Tablespace dropped.

SQL>
```

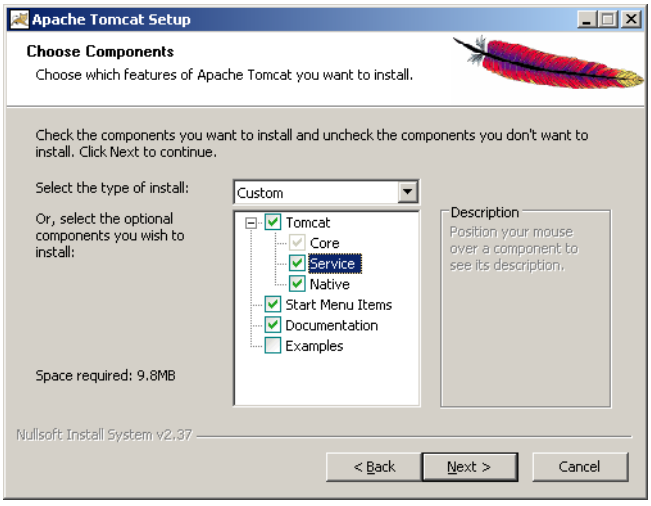
2.5. Web Application Server - Tomcat

Running IUCLID 5 in a web application server allows multiple users to access a database at the same time over a network. Alternative web application servers to Tomcat might work, but they are not supported.

2.5.1. Installation of Tomcat

The installation of the Tomcat Web Application Server is described below. Download and run the Windows Service Installer of Tomcat 6.0 from http://tomcat.apache.org/. At the step *Choose Components*, select the components *Service* and *Native*, as shown below.

Figure 2.20. Choose Components

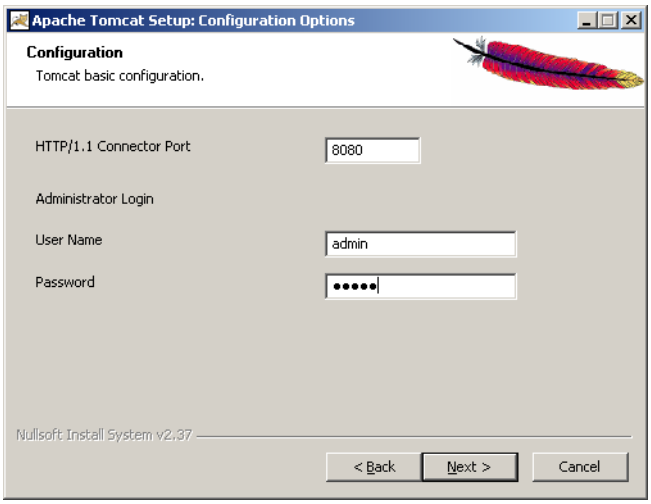

Apache Tomcat Setup
Choose Components
Choose which features of Apache Tomcat you want to install.
Check the components you want to install and uncheck the components you don't want to install. Click Next to continue.
Select the type of install:
Custom
Or, select the optional components you wish to install:
Tomcat
Core
Service
Native
Start Menu Items
Documentation
Examples
Description
Position your mouse over a component to see its description.
Space required: 9.8MB
Nullsoft Install System v2.37
< Back
Next >
Cancel

Type a name and password for the Tomcat administrator.

Important

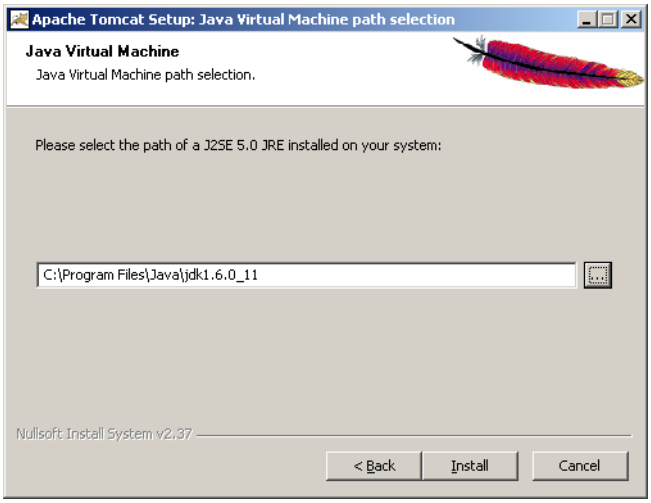
Remember these values because they are required to access the Tomcat Manager that is used to deploy, undeploy, start, and stop applications.

Figure 2.21. Configuration



Select the folder of the previously installed Java Virtual Machine

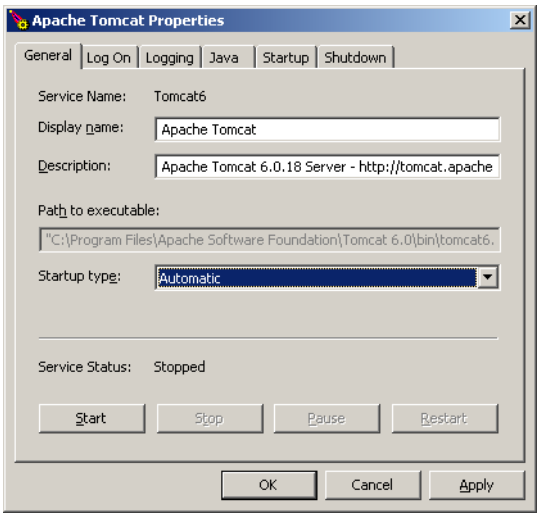
Figure 2.22. Java Virtual Machine


Apache Tomcat Setup: Java Virtual Machine path selection
Java Virtual Machine
Java Virtual Machine path selection.
Please select the path of a J2SE 5.0 JRE installed on your system:
C:\Program Files\Java\jdk1.6.0_11
Nullsoft Install System v2.37
< Back
Install
Cancel

When the installation process has finished, a new icon appears in the system tray for Tomcat, located at the bottom-right corner of the screen. Right-click on the icon and select Configure...

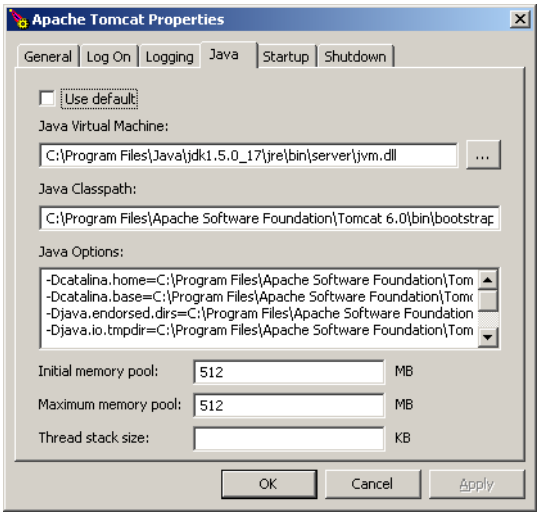
On the General tab set Automatic startup type.

Figure 2.23. General tab



On the Java tab type 512 MB for both Initial memory pool and Maximum memory pool.

Figure 2.24. Java tab

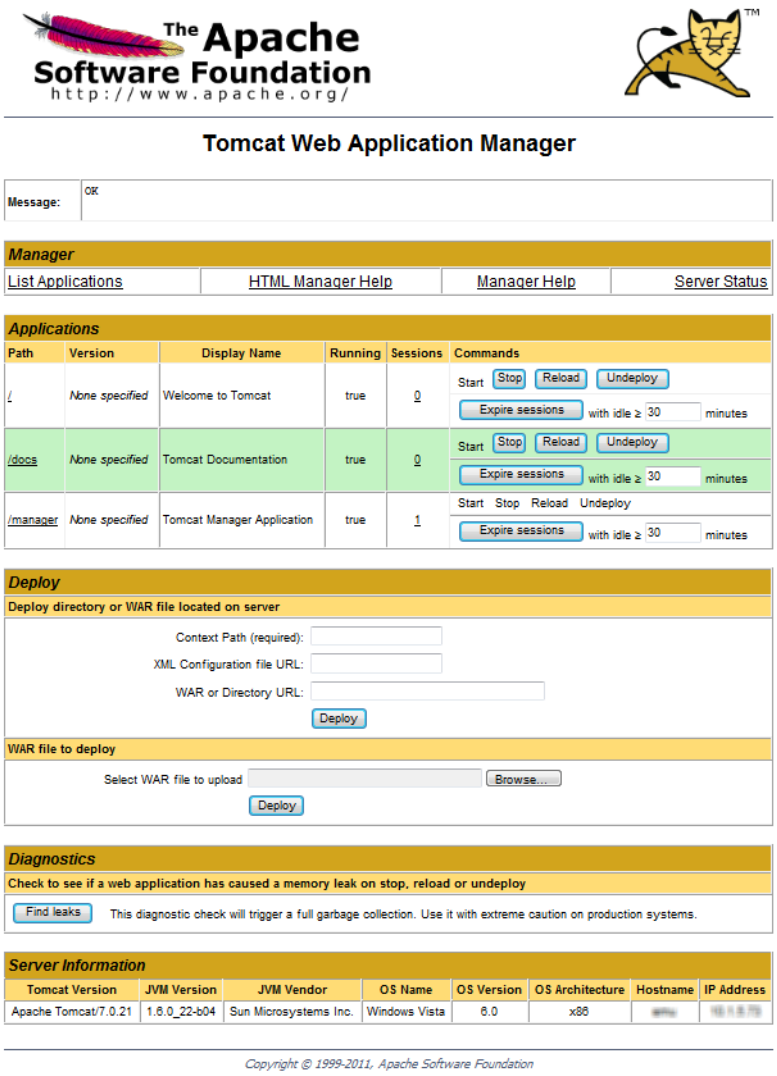


In Windows, restart the Tomcat service. This can be done from the Windows interface at start / (right click) Computer / Manage / Computer Management / Services and Applications / Services. Select the service that has a name beginning with *Apache Tomcat*. Click on Stop the Service followed by Start the Service.

2.5.1.1. Tomcat Manager

The installation of Tomcat, by default, includes the installation of *Tomcat Manager*. This is a web application that provides a means of dynamically managing web applications without having to shutdown the Tomcat web application server itself. It provides a convenient way of managing the IUCLID 5 web application in a distributed environment. To gain access to Tomcat Manager, point a web browser to the address http://localhost:8080/manager/html/. Log in to Tomcat Manager as an administrator using the username and password given during the installation of Tomcat. On logging in, the screen shown is a list of the web applications currently deployed in Tomcat. Immediately after a fresh default installation of Tomcat, the following screen is shown.

Figure 2.25. IUCLID 5 Tomcat Manager default administrator screen immediately after installation



Before attempting to deploy IUCLID 5, check the memory settings for Tomcat. To do that using Tomcat Manager, from the page shown above, click on the link Server Status and then check the field JVM. The value of *Max memory* should be at least 495 MB. Deploying IUCLID 5 in Tomcat is described in the next section.

2.5.2. Deployment in Tomcat

Deployment is the term used for the process of installing a web application into a web application server.

The web application of IUCLID 5 is published in the form of a web application archive (WAR) which is a file with extension `war`. It is available from the IUCLID website [http://iuclid.eu/], packaged into a file named `iuclid5<version>_server_<date>.zip`. Download the ZIP file from the web site. Unzip it, and then unzip an archive within it named `server.zip`. Inside there is a file named `i5server.war`. That is the file to be deployed.

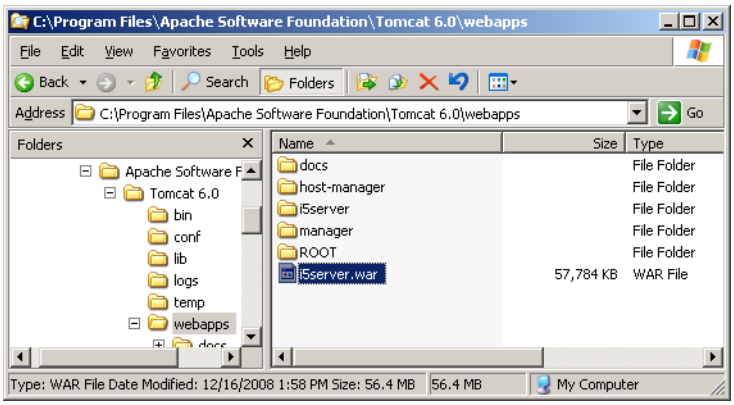
Deployment of a web application into Tomcat can be done in two ways:

- Statically - the web application is set up whilst the web application server Tomcat is not running.

- Dynamically - one or more web applications can be managed whilst the web application server Tomcat is still running. This allows IUCLID 5 to be installed on an instance of Tomcat without needing to have a break in service for any other web applications that are running on the same instance of Tomcat.

In this installation manual, only the dynamic deployment is described. However, the static deployment may be used instead. The deployment of a web application on Tomcat is described in detail on the web page Tomcat deployment [http://tomcat.apache.org/tomcat-5.5-doc/deployer-howto.html]. In essence, the deployment of IUCLID 5 consists of copying the archive file `i5server.war` into a folder within the installation of Tomcat, named `webapps`. If Tomcat is running whilst the copying is done, it automatically opens the archive and copies the content into the folder `webapps`. In addition, Tomcat automatically starts the IUCLID 5 web application. An example of what the folder `webapps` looks like in the file browser of Windows, with IUCLID 5 deployed, is shown below:

Figure 2.26. IUCLID 5 deployed in Tomcat - file browser view



When IUCLID 5 is deployed in Tomcat, it is shown in the list of web applications in Tomcat Manager, as shown below. If you are unfamiliar with Tomcat Manager, see Section 2.5.1.1, “Tomcat Manager”.

Figure 2.27. IUCLID 5 deployed in Tomcat - application list in Tomcat Manager

Applications

Path	Version	Display Name	Running	Sessions	Commands
/	None specified	Welcome to Tomcat	true	0	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/docs	None specified	Tomcat Documentation	true	0	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/i5server	None specified	IUCLID5 Server	true	1	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/manager	None specified	Tomcat Manager Application	true	1	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes

Alternatively, deployment can be done using the deploy feature of the Tomcat Manager to upload a war file into Tomcat from a filesystem. However, before doing that, the configuration of Tomcat Manager should be checked and possibly adjusted for the following reason.

Warning

By default, Tomcat Manager places an upper limit on the size of the war file that can be uploaded. The default value of the limit is smaller than the size of the file `iuclid.war`. If the size limit is exceeded, the following error is given:

The server encountered an internal error () that prevented it from fulfilling this request. Exception java.lang.IllegalStateException: org.apache.tomcat.util.http.fileupload.FileUploadBase$SizeLimitExceededException: the request was rejected because its size (XXX) exceeds the configured maximum (52428800)

The solution is to increase the size of the limit, by increasing the values of the parameters *max-file-size* and *max-request-size* in the settings file `/tomcat7/webapps/manager/WEB-INF/web.xml` to values that are larger than the size of the war file. The default values are shown below:

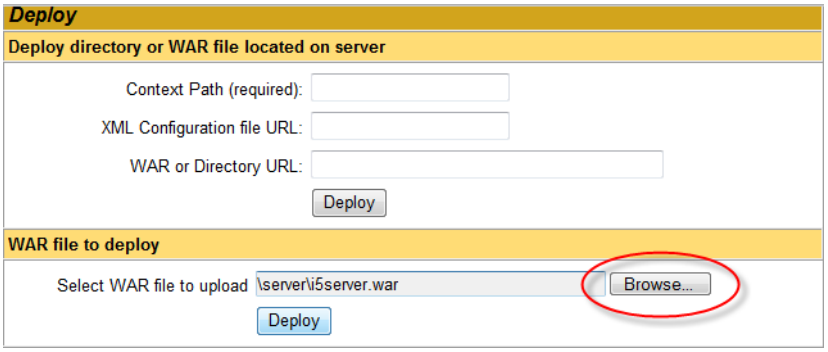
```
<multipart-config>
<!- 50MB max ->
<max-file-size>52428800</max-file-size>
<max-request-size>52428800</max-request-size>
<file-size-threshold>0</file-size-threshold>
</multipart-config>
```

An example of the new values required, for IUCLID 5.4.0, is shown below.

```
<max-file-size>80000000</max-file-size>
<max-request-size>80000000</max-request-size>
```

Once you are sure that the file size limit is large enough, in Tomcat Manager, click on the button Browse, that is under the lower of the two options deploy options, WAR file to deploy, as shown below:

Figure 2.28. Deploy IUCLID 5 in Tomcat - upload using Tomcat Manager



Browse to the file `i5server.war`, select it, and then click the button Open. Click on the lower of the buttons labelled Deploy. Check that IUCLID 5 appears within the list of web applications.

Warning

IUCLID 5 must be stopped and started for changes to the server settings to take effect, for example, to change the settings for the connection to the database. Even though Tomcat Manager can be used to stop and start only the IUCLID 5 web application, it is currently recommended that that is done only by stopping and starting Tomcat.

2.5.3. Undeployment in Tomcat - uninstall and upgrade

The IUCLID 5 web application is undeployed if it is to be uninstalled or upgraded. Tomcat Manager is particularly useful when it comes to upgrading IUCLID 5, because it provdes a reliable method of undeploying (removing) the previous version and deploying the new version, even where both archive files have the same name. In addition, this can be done without shutting down Tomcat.

To undeploy the IUCLID 5 web application using Tomcat Manager, in the application listing, click the button stop for IUCLID 5. When the value in the column Running is shown as *false*, click the button Undeploy. The IUCLID 5 web application should disappear from the application listing and its files should be deleted from the folder `webapps`.

Warning

An attempt to undeploy a web application can fail if something prevents the deletion of the application files. For example, this can happen if a user with insufficient access rights is using one of the application's files. For example, a user whose account has insufficient rights might have a settings file open. Therefore, before using undeploy in Tomcat Manager, check that no applications, and no file manager windows are open that are currently using files or folders of the web application.

In an upgrade, once the previous version of IUCLID 5 has been successfully undeployed, the new version can be deployed, as described above.

2.6. Configuring the connection to the database

The configuration of the connection from the IUCLID web application to its database is defined in the file `server.properties` that is located in the folder `webapps/i5server/WEB-INF/classes`.

The default values are for an instance of the PostgreSQL database running on the same computer as the web application server. The values for the database name, the database username/password are all set to the value *iuclid5*. If that configuration is used, on starting the IUCLID 5 web application, it will connect to the database without the need to make any changes to the configuration file. If other values are required, they must be entered into the file `server.properties`. Before editing the configuration file, ensure that no clients are connected to the IUCLID 5 web application and then stop the application using Tomcat Manager.

Important

Make sure that there are no spaces after the username and password values in the properties file.

After editing the configuration file, start the IUCLID 5 web application server using Tomcat Manager.

The IUCLID 5 server records its activities in a log file. The configuration file for the logging is `i5server.logging.properties` which is located in the folder `WEB-INF/classes`. Consult the content of this file if you encounter any errors that you cannot explain. If you are following this manual to perform a fresh installation, all the software has now been installed. What remains, is some configuration, as described in Section 2.7, “Configuring the security settings for user accounts” and Section 4.1, “Starting IUCLID 5”.

2.6.1. Database connection settings for PostgreSQL

The default configuration for PostgreSQL is shown below:

```
#
# Settings for using PostgreSQL
#
hibernate.connection.url=jdbc:postgresql://localhost:5432/iuclid5
hibernate.connection.username=iuclid5
hibernate.connection.password=iuclid5
hibernate.connection.driver_class=org.postgresql.Driver
hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect
```

In the example shown below for PostgreSQL, the database server's name is *dbserver*, the database is accepting connections on port *12345*, the database name is *chemdb* with a database user named *joe* with a password *xxxx*:

```
hibernate.connection.url=jdbc:postgresql://dbserver:12345/chemdb
hibernate.connection.username=joe
hibernate.connection.password=xxxx
```

2.6.2. Database connection settings for Oracle

The default configuration for Oracle is shown below: Uncomment the lines as required.

```
# ----------------------------
# Settings for using ORACLE 10g
# ----------------------------
#hibernate.connection.username=<username>
#hibernate.connection.password=<password>
#hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
#hibernate.connection.url=jdbc:oracle:thin:@localhost:1521:<database>
#hibernate.hbm2ddl.auto=validate
#hibernate.dialect=eu.eca.iuclid.server.system.persistence.ExtendedOracle9Dialect
#hibernate.jdbc.use_streams_for_binary=false
```

2.7. Configuring the security settings for user accounts

IUCLID 5 has features designed to control the level of security of authentication of user accounts. The level of security can be tailored to that required for the particular instance of IUCLID 5. For example, when setting passwords for their user accounts, users can be forced to enter values that have a minimum strength. The values of the parameters that determine the level of security are defined in two settings files, `server.properties` and `client.properties`, both of which are located in the folder `webapps/i5server/WEB-INF/classes/`. Changes to values take effect on restarting the **server** software of IUCLID 5. The security features are described below, grouped together by settings file.

2.7.1. User account security settings defined in `client.properties`

The settings are shown below as they appear in the settings file that is supplied with the installation of IUCLID 5. The values are shown set to the hard-coded defaults. If a line is commented out, the default value is used. A value of zero (0) disables a feature.

```
# The minimum length for a new password
password.min.length=6
# The minimum number of character sets used in the password
password.min.charsets=2
# If a secure question system is enabled
password.use.secure.question=true
```

2.7.1.1. Minimum password length

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least this number of characters. If an attempt is made to create a password with fewer characters, an informative error message is given and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum length of passwords is increased, users can still log in using existing passwords, even if they are now considered to be too short. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.7.1.2. Minimum number of character sets in passwords

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least one character from all the character sets. The value is an integer from 1 to 4. A value of 1 means only character set 1, a value of 2 means both character sets 1 and 2, etc. The four character sets are: 1 = a lowercase letter [a-z], 2 = an uppercase letter [A-Z], 3 = a digit [0-9], 4 = a non-alphanumeric symbol [!@#$%^&*-_=+].

For example, if the value is 3, a password of "AdkbScfw" is rejected for being too weak, but "AdkbSc37" is accepted because it contains at least one character from sets 1, 2 and 3.

If an attempt is made to create a password that does not comply, an informative error message is given, and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum number of character sets allowed within passwords is increased, users can still log in using existing passwords, even if they are now considered to contain too few character sets. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.7.1.3. Security question

This feature is designed to allow an alternative method of user authentication to the user name/password combination. It can help to reduce the resources required for user management by preventing account blocking due to forgotten passwords. Each user can define their own security question and a secret answer. This is done from the graphical user interface of the client, after the user has logged in. A user can log in by answering their question correctly, instead of supplying the password. The question is answered via a link on the log in page, Forgot your password?. The feature is turned on or off for the whole instance of IUCLID 5 using a value of `true` or `false`.

2.7.2. User account security settings defined in `server.properties`

The settings are shown below as they appear in the settings file that is supplied with the installation of IUCLID 5. The values are shown set to the hard-coded defaults. If a line is commented out, the default value is used. A value of zero (0) disables a feature. A suspended account can be un-suspended by a user with user-management rights.

```
# Account expiry in days. A value of zero (0) disables the feature
account.expiry=180
# Password expiry in days. Zero (0) disables the feature.
password.expiry=90
# Max number of attempts before the account is disabled. Zero (0) disables the feature.
max.failed.login.attempts=3
# Max number of attempts to answer the reset question.
max.failed.answer.attempts=3
```

2.7.2.1. Account expiry period

This feature is used to automatically suspend an account that has not been used for a long time. If the period between two successive successful log in attempts exceeds the value, the account is suspended.

2.7.2.2. Password expiry period

This feature is used to prevent users from using the same password for long periods. It defines the life-span of a password. After the password has been in use for the period, the user is prompted to change the password when they next log in. The period is counted from the time of first logging in to the account, then after that, from the time of changing the password.

2.7.2.3. Maximum number of attempts to log in

This feature is used to prevent the combination of user name and password from being obtained by trial and error. The value is the maximum number of successive unsuccessful attempts there can be to log in to an account before it is suspended.

2.7.2.4. Maximum number of attempts to answer the security question

This feature is used to prevent the security question from being answered by trial and error. The value is the maximum number of successive unsuccessful attempts there can be to answer the security question before the account is suspended.

Chapter 3. Upgrade

This document describes the update process from only IUCLID 5.3.x. The version can be seen from within the interface of IUCLID 5. To see the version, start IUCLID 5, log-in, then click *Help* and select *About*. To upgrade from IUCLID 5.2 or earlier to IUCLID 5.4, first upgrade to IUCLID 5.3.2, then follow the steps in this chapter. The software packages and instructions required to upgrade to IUCLID 5.3.2 are available on the IUCLID web site.

Before starting the upgrade, it is important to back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up functionality of the database. Making only a copy of the file system on which IUCLID is installed is *not* recommended as a means of backing-up.

Warning

The built-in back-up functionality of IUCLID 5.3.1 is known to output files in which the user accounts cannot be used on restore. If you wish to use the built-in back-up functionality on data in an installation of IUCLID 5.3.1, first upgrade it to IUCLID 5.3.2. The built-in back-up functionality in IUCLID 5.3.2 does not suffer from this problem.

The migration process changes the IUCLID database such that it can no longer be used with previous versions of the IUCLID application. Therefore, if you would like to be able to continue to use a database with the previous version of IUCLID, do not run the migration tool on that particular database. Either perform a fresh installation of the new version of IUCLID and transfer the data across to it using Back-up/Restore, or perform the upgrade and migration on a duplicate of the old database. If two versions of IUCLID are to be run on the same computer, appropriate database settings must be used to avoid conflicts. Do not run two distributed versions of IUCLID at the same time on the same computer.

3.1. Upgrade and migration of data from IUCLID 5.3.x to IUCLID 5.4

There are various different ways to manage a Tomcat web application server, as referred to in the section of this manual Deployment of IUCLID 5. The following instructions are intended to give a representative example of how the IUCLID 5 software can be upgraded and the data migrated from IUCLID 5.3.x to 5.4.

1. Back-up the database. Use the built-in back-up functionality of IUCLID 5, and/or the back-up function of the database software, for example PostgreSQL. The built-in backup feature is accessible by only the user `SuperUser`, from the menu File / Administrative tools / Backup.
2. Close all clients for IUCLID 5.
3. Use the application Tomcat Manager to stop the IUCLID 5.3.x web application.
4. Copy the configuration file for IUCLID 5.3.x, `server.properties`, into a backup folder. Note that the plugins for IUCLID 5.3.x are not compatible with IUCLID 5.4. Therefore, they must *not* be copied over to the new installation.

   For example:

   copy `%TOMCAT%\webapps\i5server\WEB-INF\classes\server.properties`

   to

   `e:\backup\server.properties`
5. Use the application Tomcat Manager to undeploy the IUCLID 5.3.x web application.
6. Use the application Tomcat Manager to deploy the IUCLID 5.4 web application.

7. Stop Tomcat.

8. Copy any values that are specific to your system from the previous version of the file `server.properties` to that supplied with the new version of IUCLID 5. Ensure that the new values for the database connection are those for the database of the system to be upgraded.

Tip

IUCLID 5.3.2 was the first version of IUCLID 5 for which the file `client.properties` contained values that might need to be changed. The file is in the same folder as the file `server.properties`. The settings are for the security features for user accounts. See Section 2.7, “Configuring the security settings for user accounts” for more details.

9. Note that if the Oracle database is used, the file `server.properties` must contain the following entry. Add it or edit the existing entry if required.

```
hibernate.connection.driver_class=oracle.jdbc.OracleDriver
```

10. If the database is an Oracle database, please note that the driver for Java is no longer supplied with the IUCLID 5 installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Java 1.6 and Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`.

11. The database and all the data it contains are migrated from the previous to the new version by running IUCLID 5.4 in update mode, only once. IUCLID 5.4 is instructed to start in update mode by the line shown below in the file `server.properties`.

```
database.update.startup=true
```

The line is supplied, although commented out, in the file `server.properties` in the installation package for IUCLID 5.4. To run in update mode, the line must be either uncommented or added as shown above.

12. To begin the migration, start Tomcat. This automatically starts the new version of the IUCLID 5 web application.

Dependent on the quantity of data in the database, and the system resources available, the migration process can take from minutes to many hours. It is essential that the migration process is not interrupted. The progress of the migration can be monitored from the log files `i5server.log` and `iuclidMT.log` . The default location of these files is on the top level directory of the Tomcat installation. The file `i5server.log` contains statements about the start and end of the migration process. The file `iuclidMT.log` contains full details. If you need to know what happened during the migration process, check those files first.. At the start of the process the following entry is shown:

```
integration.database.scripts.ScriptUtils - Checking Database Status...
(eu/eca/iuclid/server/integration/database/scripts/migrate_schemav50_
to_schemav51.xml)
integration.database.scripts.ScriptUtils - Upgrading table
integration.database.scripts.ScriptUtils -

************************************

Database changes are being applied now.
This process might, depending on the size of your database, take some time
(several minutes to perhaps hours). Please do NOT shutdown the system as this
might result in an inconsistent database state.
```

As the migration proceeds, details of which data are being migrated are written to `iuclidMT.log`. The end of a successful migration is indicated by the following entry:

```
integration.database.scripts.ScriptUtils - Database update successfully finished.
integration.database.scripts.ScriptUtils - Checking Database Status...
(eu/eca/iuclid/server/integration/database/scripts/
migrate_schemav51_patch.xml)
integration.database.scripts.ScriptUtils - Upgrading table
integration.database.scripts.ScriptUtils - Database is up to date.
```

If the migration is interrupted, or fails, for whatever reason, the database must be restored from the back-up and the migration started again.

13. When the migration finishes successfully, stop the new version of the IUCLID 5 web application by stopping Tomcat.

14. Set IUCLID 5 to start *not* in its update mode by commenting out the line edited previously:

```
#database.update.startup=true
```

15. Start Tomcat.

16. Run the IUCLID 5 client in the same way as before the upgrade. The initialisation process is not required. All of the data that was present before the upgrade should be present in the new system. Therefore, it should be possible to log in to any of the user accounts that were present prior to the upgrade.

17. Log in to the IUCLID 5 client as one of the users that was present before the upgrade.

18. Confirm that the version of IUCLID 5 is the new, expected version. This can be seen from the menu Help / About.

19. Confirm that the data from the previous version has been successfully migrated to the new version.

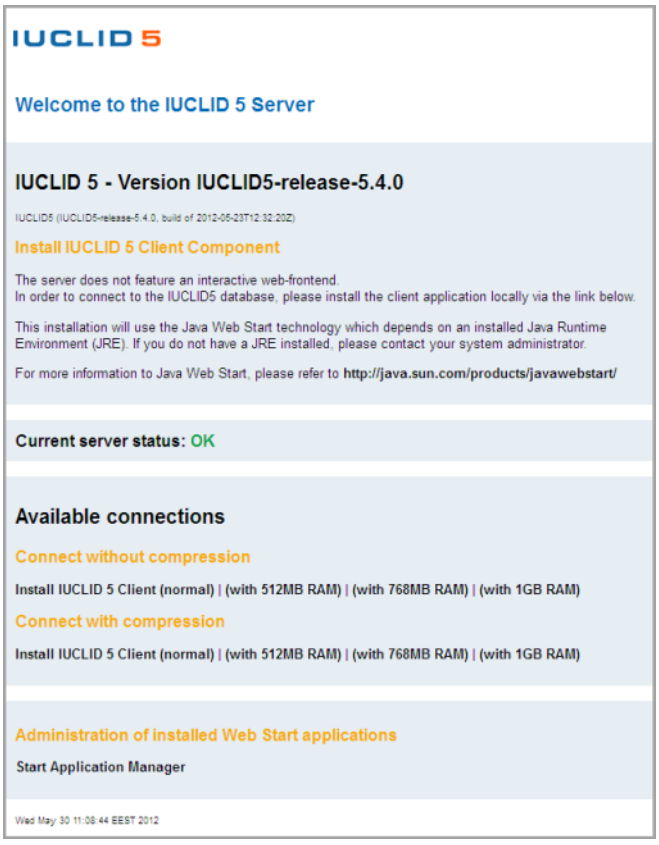
Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a back-up that was made using the built-in back-up function of IUCLID. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from back-up, make sure that the back-up files are accessible from the system on which IUCLID will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Connect to the application with a browser by entering the address *http://<address of your server>:8080/i5server*. An example of the page displayed is shown below.

Figure 4.1. Example default page for Java Web Start of IUCLID 5


IUCLID 5
Welcome to the IUCLID 5 Server
IUCLID 5 - Version IUCLID5-release-5.4.0
IUCLID5 (IUCLID5-release-5.4.0, build of 2012-05-23T12:32:20Z)
Install IUCLID 5 Client Component
The server does not feature an interactive web-frontend.
In order to connect to the IUCLID5 database, please install the client application locally via the link below.
This installation will use the Java Web Start technology which depends on an installed Java Runtime Environment (JRE). If you do not have a JRE installed, please contact your system administrator.
For more information to Java Web Start, please refer to http://java.sun.com/products/javawebstart/
Current server status: OK
Available connections
Connect without compression
Install IUCLID 5 Client (normal) | (with 512MB RAM) | (with 768MB RAM) | (with 1GB RAM)
Connect with compression
Install IUCLID 5 Client (normal) | (with 512MB RAM) | (with 768MB RAM) | (with 1GB RAM)
Administration of installed Web Start applications
Start Application Manager
Wed May 30 11:08:44 EEST 2012

The page shown above page contains links that use Java Web Start technology to start a client that connects to the IUCLID server and displays IUCLID 5's graphical user interface (GUI) on the client machine. In the example shown above, the link under the text "IUCLID 5 Client (with 1GB RAM)" has already been followed. The difference between the links in the above page is that each link passes different parameters to the IUCLID 5 server. The options included are for varying amounts of memory to be allocated to IUCLID 5 and for different types of data compression to be employed in the connection to the server. If IUCLID 5 runs slower than you would like and you have the available memory, select a link for a larger amount of RAM. The client can be run directly from a browser or by first downloading

a file from one of the links and running that. Depending on your browser settings, when you click on one of the links above you will see either a dialogue box, or IUCLID 5 will run and you will see the login page. The browser dialogue asks whether you would like to save a file or run it straight away. The choice is yours. A convenient way to access IUCLID 5 is to download one of the files from the default page, save it to the desktop of your local machine used to access IUCLID 5 and give it the IUCLID 5 icon that comes with the installation. Double clicking on the icon then launches the IUCLID 5 GUI. Once you see the login page, you are ready to go walk through the First steps wizard, as described in the next section.

4.2. First steps wizard

When you start IUCLID 5 for the first time, the *First steps* wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 End-user Manual.

Important

This wizard allows a single user account to be created, per run. This user is in addition to the *SuperUser* account that comes with the installation. It is essential to have at least one user account in addition to *SuperUser* because *SuperUser* should be used only for the special tasks that only it can carry out. See the IUCLID 5 End-user Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 End-user Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 End-user Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the *SuperUser*. This is done from the file menu within IUCLID 5 **Administrative tools** / **Initialise**.

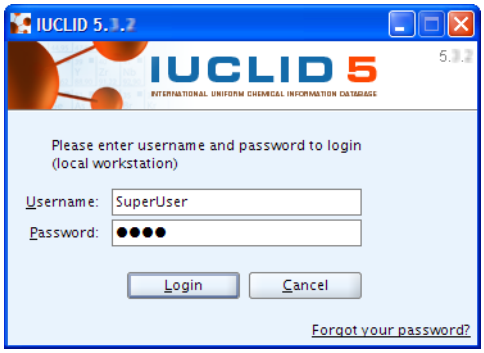
When starting the IUCLID 5 for the first time, the only user available is an administrator named *SuperUser*. Log in as *SuperUser* by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

Password: root

Note

Do not click on the link **Forgot your password?** if the *First steps* wizard is being run for the first time on this database. This feature can work only after the wizard has been completed. The use of the feature **Forgot your password?** is explained later in this wizard, at step 3.



The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

Figure 4.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the **Next** button.

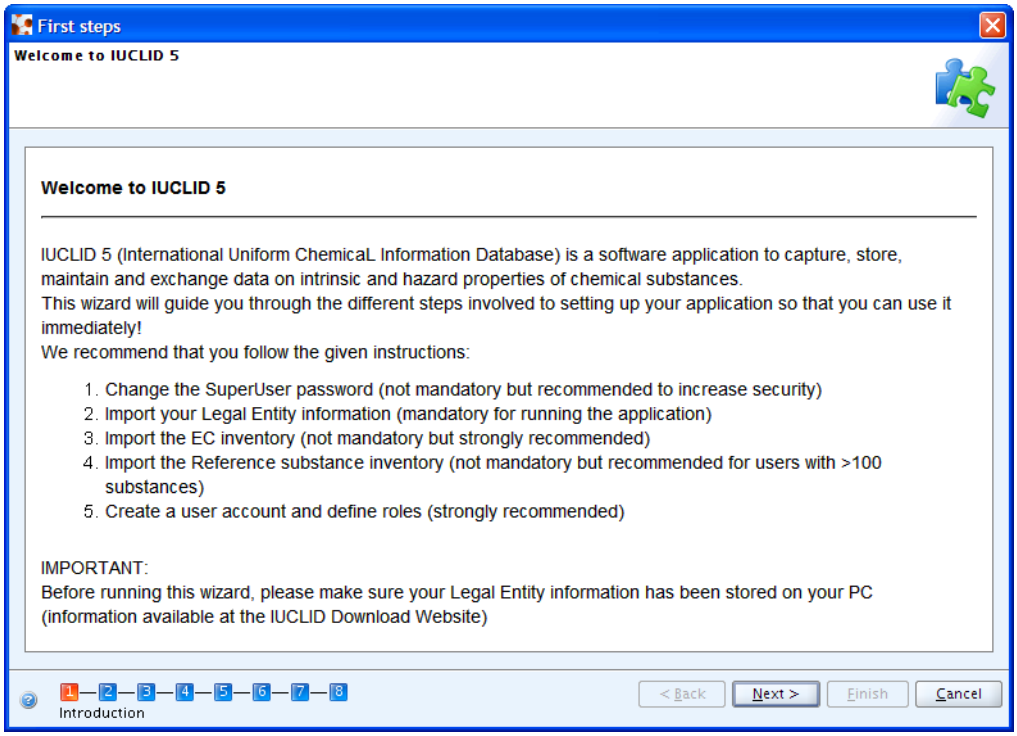

First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately!
We recommend that you follow the given instructions:
1. Change the SuperUser password (not mandatory but recommended to increase security)
2. Import your Legal Entity information (mandatory for running the application)
3. Import the EC inventory (not mandatory but strongly recommended)
4. Import the Reference substance inventory (not mandatory but recommended for users with >100 substances)
5. Create a user account and define roles (strongly recommended)
IMPORTANT:
Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
1 2 3 4 5 6 7 8
Introduction
< Back
Next >
Finish
Cancel

Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button `New Installation`as shown below and continue to the next step.

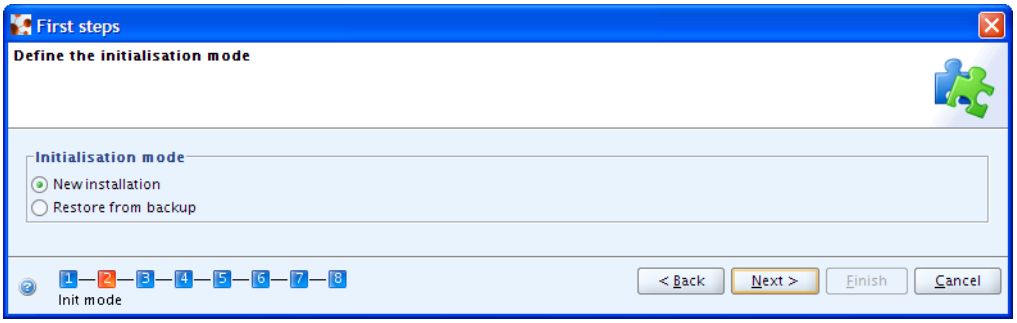
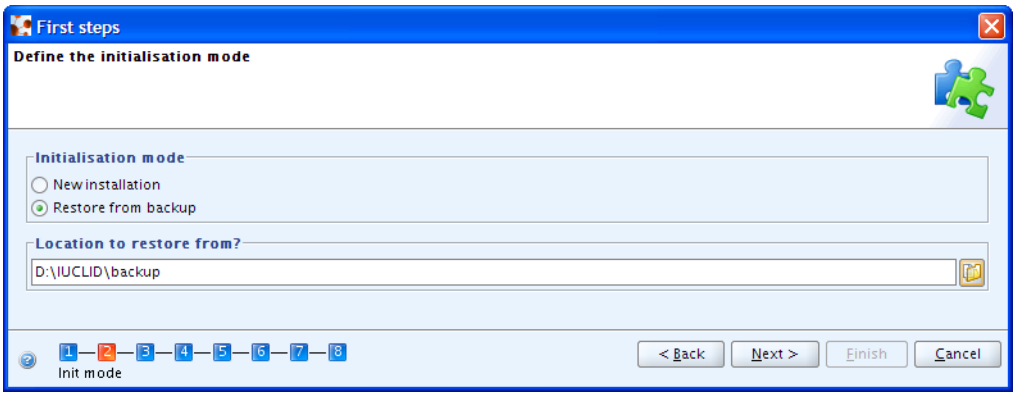


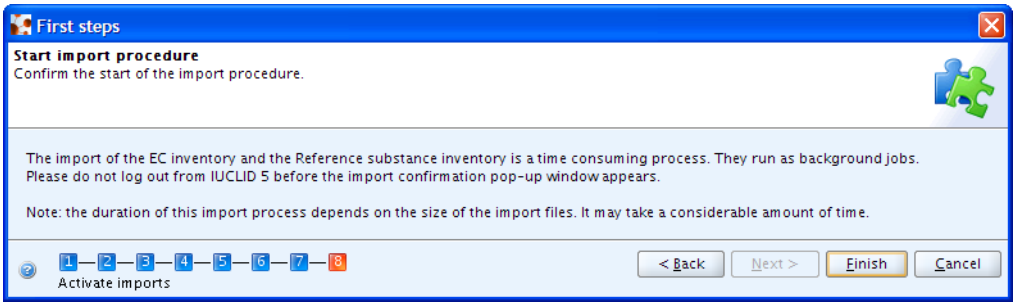
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button `Restore from backup` then enter the directory containing the backup files as shown in the example below.



Click **Next**. The wizard jumps to its last step, where the importation of data is started, as shown below.

Figure 4.5. Restoration from a back-up - Step 8 - Activate imports


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

The import may take some time. Click *Finish*. When the restoration is complete, the following screen is shown.

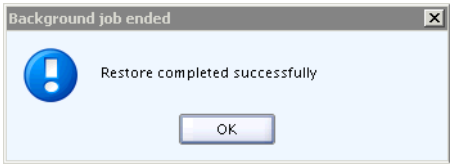
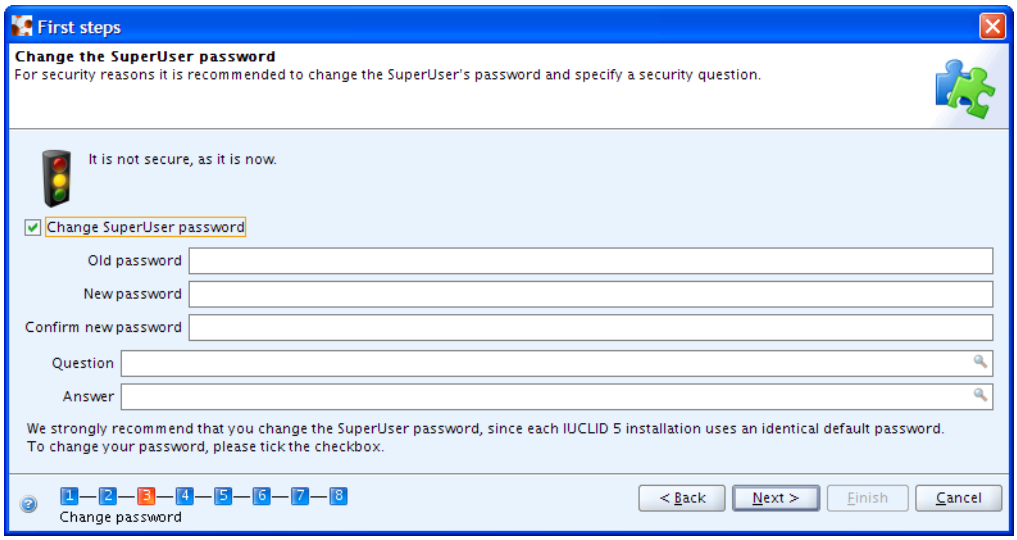


Figure 4.6. Step 3 of the First steps wizard - Change password

If the password for *SuperUser* has never been changed from its default value of *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box `Change SuperUser password` , enter the current password, and then the new password, and then the new password again.

To proceed, click the button **Next**.


First steps
Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password and specify a security question.
It is not secure, as it is now.
Change SuperUser password
Old password
New password
Confirm new password
Question
Answer
We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.
1 2 3 4 5 6 7 8
Change password
< Back
Next >
Finish
Cancel

Tip

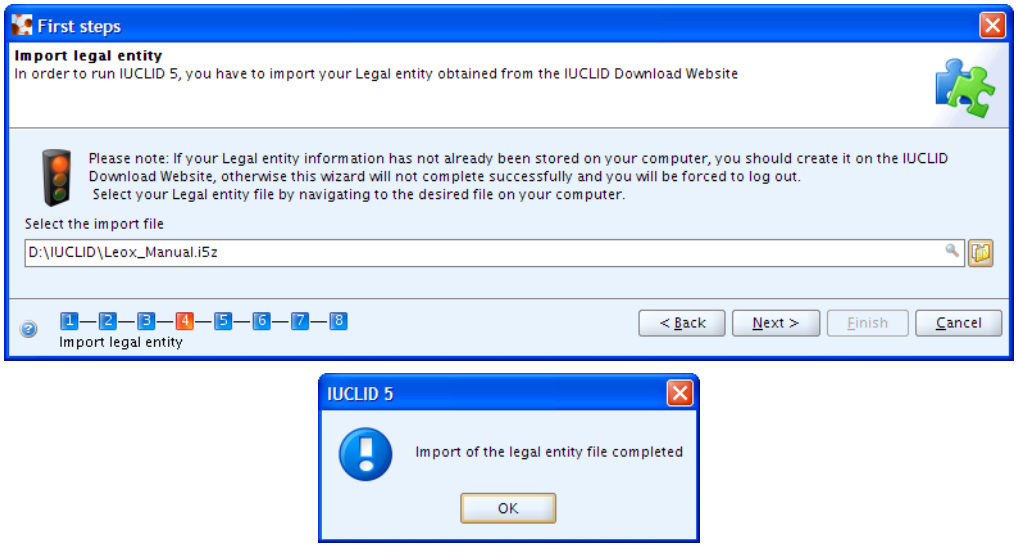
IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

Tip

IUCLID 5 has a feature that allows a user to log in by answering a security question, instead of providing the password for the account. Users define their own questions and answers from within their own accounts. However, the SuperUser is a special case, because the question and answer can be defined before logging in for the first time. The question and answer are entered into the fields shown above in step 3 of the wizard. To use the feature to log in, a user clicks on the link **Forgot your password?** which is situated at the bottom right of the login page.

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 End-user Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field Select the import file. Click the **Next** button. The Legal entity is imported immediately.


First steps
Import legal entity
In order to run IUCLID 5, you have to import your Legal entity obtained from the IUCLID Download Website
Please note: If your Legal entity information has not already been stored on your computer, you should create it on the IUCLID Download Website, otherwise this wizard will not complete successfully and you will be forced to log out.
Select your Legal entity file by navigating to the desired file on your computer.
Select the import file
D:\IUCLID\Leox_Manual.i5z
1 2 3 4 5 6 7 8
Import legal entity
< Back
Next >
Finish
Cancel
IUCLID 5
Import of the legal entity file completed
OK

Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

Figure 4.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 End-user Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

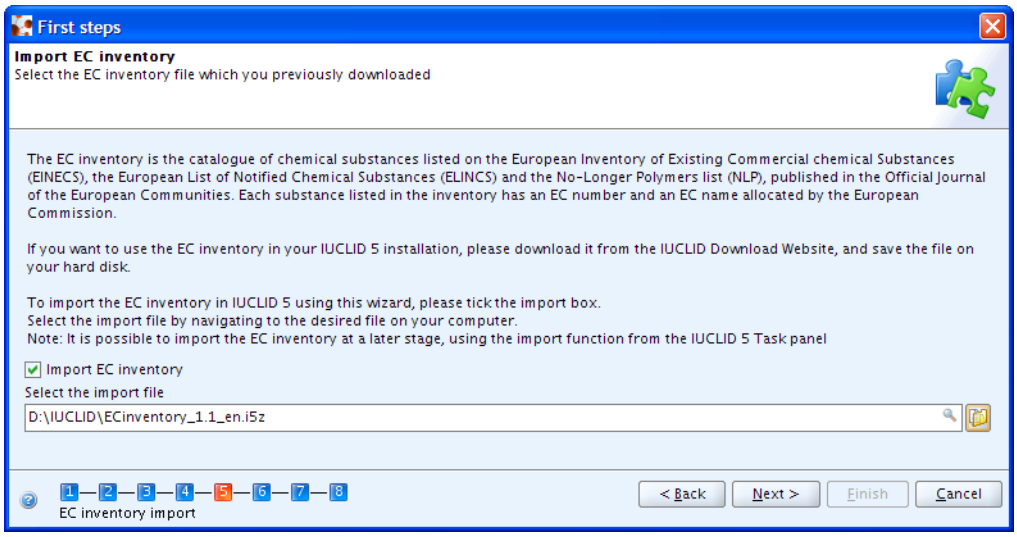
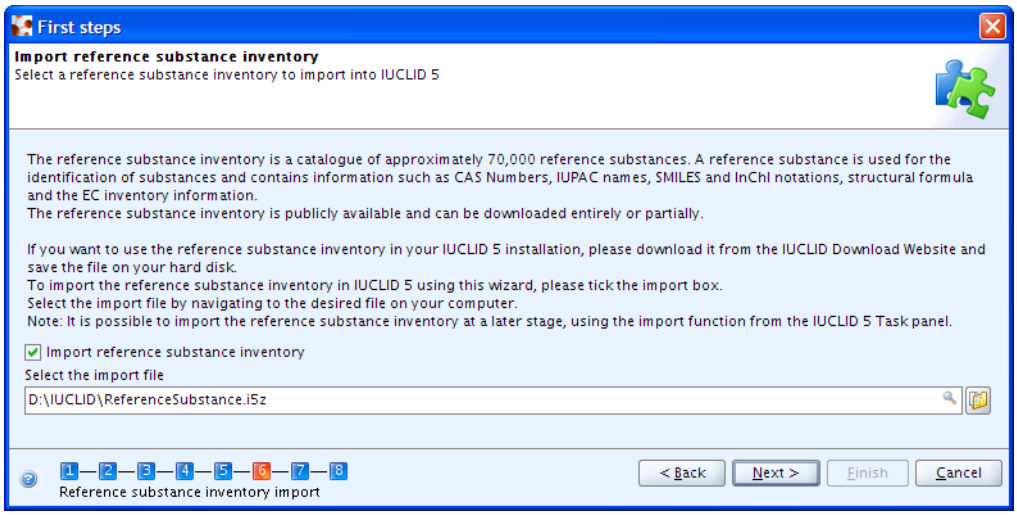

First steps
Import EC inventory
Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journal of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
Import EC inventory
Select the import file
D:\IUCLID\ECinventory_1.1_en.i5z
1 2 3 4 5 6 7 8
EC inventory import
< Back
Next >
Finish
Cancel

Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 End-user Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a long time. The import of the Reference substance inventory itself can take **up to several hours**.

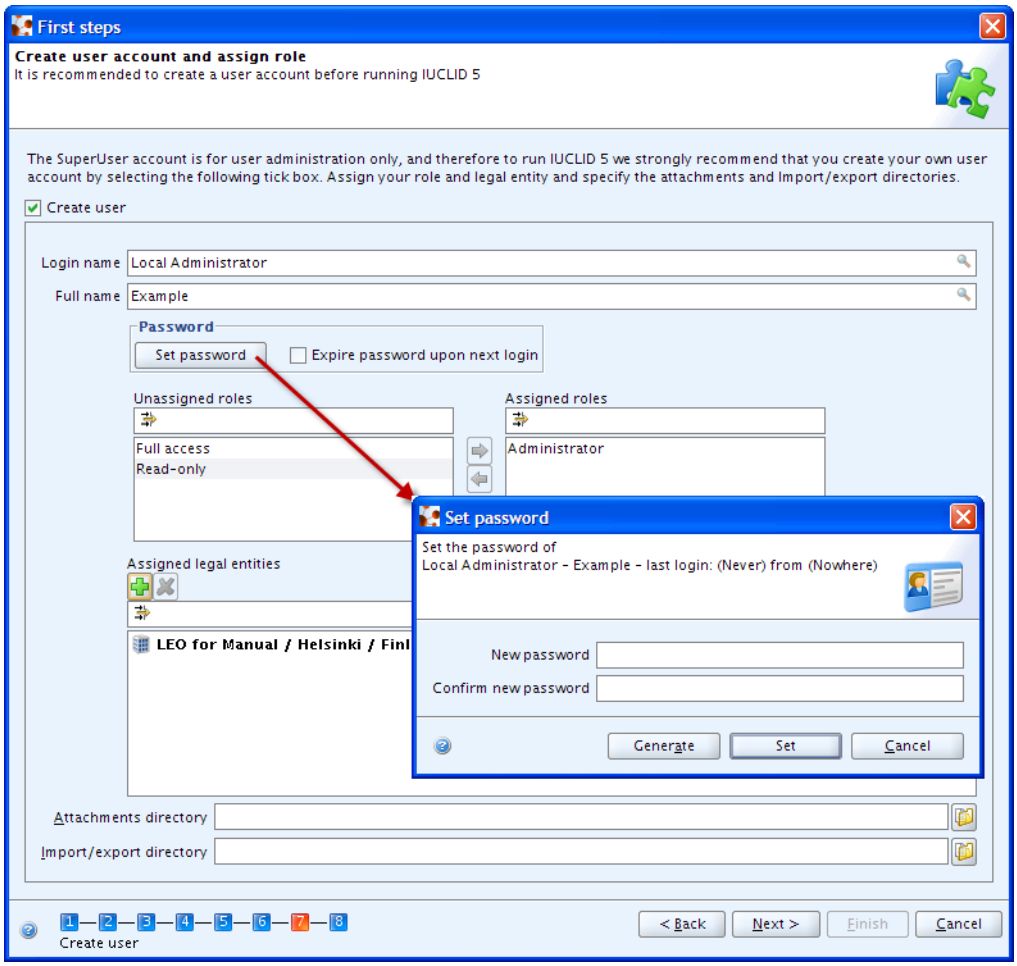

First steps
Import reference substance inventory
Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information.
The reference substance inventory is publicly available and can be downloaded entirely or partially.
If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk.
To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel.
Import reference substance inventory
Select the import file
D:\IUCLID\ReferenceSubstance.i5z
1 2 3 4 5 6 7 8
Reference substance inventory import
< Back
Next >
Finish
Cancel

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set,* a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.


First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directories.
Create user
Login name
Local Administrator
Full name
Example
Password
Set password
Expire password upon next login
Unassigned roles
Full access
Read-only
Assigned roles
Administrator
Assigned legal entities
LEO for Manual / Helsinki / Finl
Set password
Set the password of
Local Administrator - Example - last login: (Never) from (Nowhere)
New password
Confirm new password
Generate
Set
Cancel
Attachments directory
Import/export directory
1 2 3 4 5 6 7 8
Create user
< Back
Next >
Finish
Cancel

- Select the checkbox `Create user`.

  Fill in all the fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions. In a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default.

- Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Click *Set password* to define a password.

Tip

IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file

within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

Tip

If you want a use-once password that is reasonably hard to guess and that definitely conforms to the password policy, you can let IUCLID 5 make one for you, by clicking on the button *Generate*. It will be displayed in a new window for you to make a record of it. On closing that window it will be automatically entered into the fields *New password* and *Confirm new password*.

- Ticking the box *Expire password upon next login* forces whoever logs in to the account first to set their own password.

- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default).

Tip

It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 End-user Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.

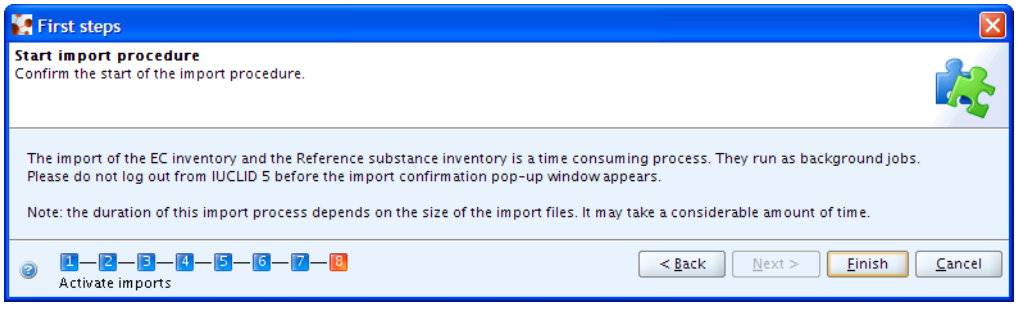
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 End-user Manual.

- Click the **Next** button

Figure 4.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

4.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 User Manual. Individual users can connect to the IUCLID 5 server using Java Web Start technology, as described in section 3.1 of this document. A convenient way to achieve that is for users to save onto their desktop, one of the files downloaded from the default Java Web Start page. The user would launch IUCLID 5 by simply double-clicking on the icon on his or her desktop. Alternatively, the users could be supplied with the URL *http://<address of your server>:8080/i5server* and instructions on which link to use.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID is a manual process. IUCLID can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.